10/10/2007,10595126IIa.trn

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PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
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FILE 'HCAPLUS' ENTERED AT 09:20:35 ON 25 SEP 2007
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.60	174.91

=> file reg
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.60	174:91

FILE 'REGISTRY' ENTERED AT 09:20:43 ON 25 SEP 2007
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STRUCTURE FILE UPDATES: 24 SEP 2007 HIGHEST RN 947820-54-4
DICTIONARY FILE UPDATES: 24 SEP 2007 HIGHEST RN 947820-54-4

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and
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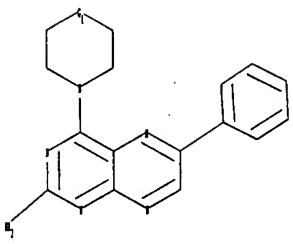
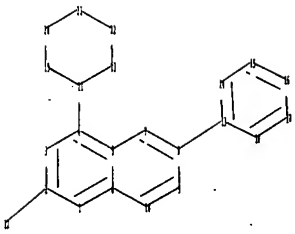
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10595126IIa.str





chain nodes :
12
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 13 14 15 16 17 18 19 20 21 22 23
chain bonds :
2-12 4-11 8-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-19 11-23 13-14 13-18 14-15 15-16 16-17 17-18 19-20 20-21 21-22 22-23
exact/norm bonds :
2-12 4-11 8-13 11-19 11-23 19-20 20-21 21-22 22-23
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 13-14 13-18 14-15 15-16 16-17 17-18
isolated ring systems :
containing 1 : 11 : 13 :

G1:CH2,O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom

L5 STRUCTURE UPLOADED

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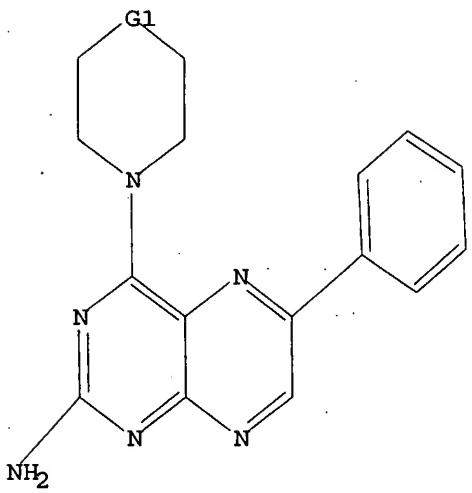
L5 HAS NO ANSWERS
L5 STR



G1 CH2,O,S

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 09:21:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        11 TO ITERATE

100.0% PROCESSED        11 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           22 TO      418
PROJECTED ANSWERS:               3 TO      163

L6             3 SEA SSS SAM L5

=> s l5 full
FULL SEARCH INITIATED 09:21:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       235 TO ITERATE

100.0% PROCESSED       235 ITERATIONS                               58 ANSWERS
SEARCH TIME: 00.00.01

L7            58 SEA SSS FUL L5

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                             172.10     347.01

FILE 'HCAPLUS' ENTERED AT 09:21:08 ON 25 SEP 2007
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FILE COVERS 1907 - 25 Sep 2007 VOL 147 ISS 14
FILE LAST UPDATED: 24 Sep 2007 (20070924/ED)

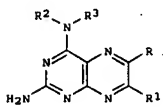
New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7
L8 14 L7

=> d ed abs ibib hitstr tot

L8 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Jun 2005
GI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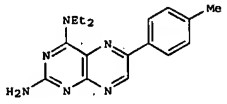

II

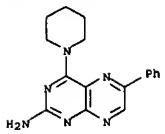
AB The title compds. I [wherein R = H, (un)substituted alkyl, alkoxy, etc.; R1 = H, Ph, alkyl, etc.; R2 and R3 = independently alkyl, PhCH2, etc.] or pharmaceutically acceptable salts thereof are prepared as NO synthetase inhibitors for the prevention and treatment of diseases caused by NO level rise. For example, the compound II was prepared II inhibited NO generation with ID50 of 14.85 μM.

ACCESSION NUMBER: 2005:561514 HCAPLUS
DOCUMENT NUMBER: 143:211928
TITLE: Preparation of Pteridine derivatives as nitric oxide synthase inhibitors
INVENTOR(S): Yao, Qizheng
PATENT ASSIGNEE(S): China Pharmaceutical University, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, No pp. given
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

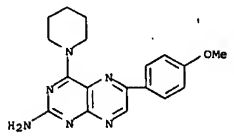
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1546491	A	20041117	CN 2003-10106588	20031210
PRIORITY APPLN. INFO.:			CN 2003-10106588	20031210

OTHER SOURCE(S): CASREACT 143:211928; MARPAT 143:211928
IT 247913-60-6P 247913-61-7P 862503-58-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pteridine derivs. as nitric oxide synthase inhibitors)
RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

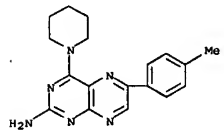
L8 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



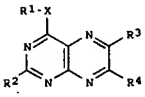
RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 862503-58-0 HCAPLUS
CN 2-Pteridinamine, 6-(4-methylphenyl)-4-(1-piperidinyl)- (CA INDEX NAME)



L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 25 Mar 2005
GI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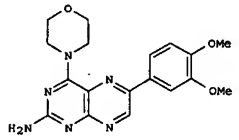

II

AB Pteridine derivs. of formula I [X = O, SOm; m = 0-2; R1 = alkyl, cycloalkyl, aryl, arylalkyl, heterocyclyl, etc.; R2 = amino, acylamino, carbamoyl, ureido, etc.; R3, R4 = H, halo, alkyl, carboxyalkyl, arylamino, etc.; R3R4 = alkylene, etc.] are prepared for the manufacture of a medicament for the prevention or treatment of septic shock and TNF-α related disorders. Thus, II was prepared, and had IC50 of 0.4 μM against TNF-α.

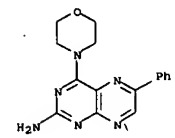
ACCESSION NUMBER: 2005:259882 HCAPLUS
DOCUMENT NUMBER: 142:336393
TITLE: Preparation of pteridine derivatives for the treatment of septic shock and TNF-α-related diseases.
INVENTOR(S): Waer, Mark Jozef Albert; Herdewijn, Piet Andre Maurits Maria; De Jonghe, Steven Cesar Alfons; Marchand, Arnaud Didier Marie; Yuan, Lin; El Hassane, Sefrioui
PATENT ASSIGNEE(S): 4 Aza Bioscience Nv, Belg.
SOURCE: PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005025574	A2	20050324	WO 2004-EP10198	20040913
WO 2005025574	A3	20050630		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
GB 2405793	A	20050316	GB 2003-21384	20030912

L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

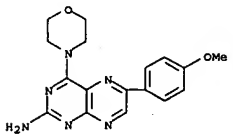
GB 2413324	A	20051026	GB 2004-8955	20040422
AU 2004271721	A1	20050324	AU 2004-271721	20040913
CA 2534549	A1	20050324	CA 2004-2534549	20040913
EP 1663244	A2	20060607	EP 2004-765120	20040913
EP 1663244	B1	20070815		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
US 2007004721	A1	20070104	US 2006-595161	20060310
PRIORITY APPLN. INFO.:			GB 2003-21384 A	20030912
			GB 2004-8955 A	20040422
			WO 2004-EP10198 W	20040913

OTHER SOURCE(S): CASREACT 142:336393; MARPAT 142:336393
IT 247913-58-2P 247913-59-3P 247913-60-6P
247913-61-7P 278800-06-9P 278800-07-0P
278800-08-1P 278800-09-2P 278800-18-3P
847756-41-6P 847756-42-7P 847756-43-8P
847756-44-9P 847756-45-0P 847756-46-1P
847756-47-2P 847756-48-3P 847756-50-7P
847756-51-8P 847756-52-9P 847756-53-0P
847756-54-1P 847756-55-2P 847756-56-3P
847756-57-4P 847756-58-5P 847756-59-6P
847756-60-9P 847756-61-0P 847756-62-1P
847756-63-2P 847756-64-3P 847756-65-4P
847756-66-5P 847756-68-7P 847756-69-8P
847756-70-1P 847756-71-2P 847756-72-3P
847756-73-4P 847756-74-5P 847756-75-6P
847756-76-7P 847756-82-5P 848415-15-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pteridine derivs. for treatment of septic shock and TNF-α-related diseases)
RN 247913-58-2 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-phenyl- (9CI) (CA INDEX NAME)

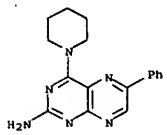


RN 247913-59-3 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

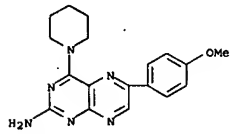
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

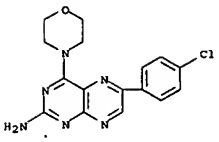


RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

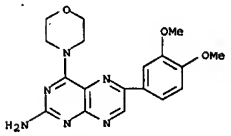


RN 278800-06-9 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 278800-07-0 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)



RN 278800-08-1 HCAPLUS
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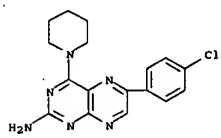
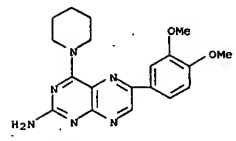
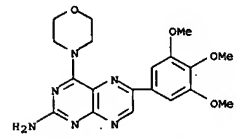


RN 278800-09-2 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

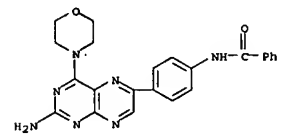
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 278800-18-3 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

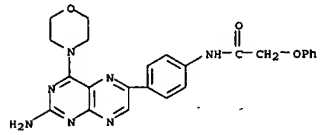


RN 847756-41-6 HCAPLUS
CN Benzamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

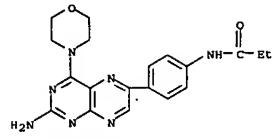


RN 847756-42-7 HCAPLUS
CN Acetamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-2-phenoxy- (CA INDEX NAME)

L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-43-8 HCAPLUS
CN Propanamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)



RN 847756-44-9 HCAPLUS
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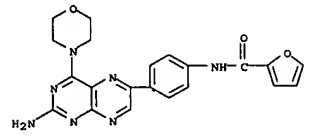
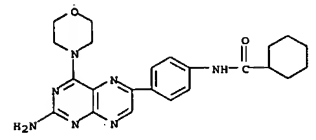


RN 847756-45-0 HCAPLUS
CN Cyclohexanecarboxamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)



L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 847756-46-1 HCAPLUS
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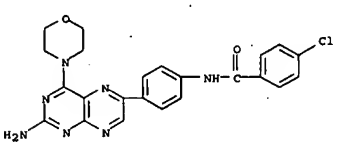
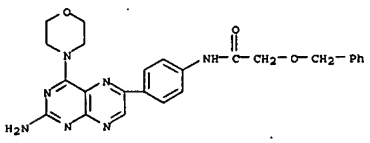
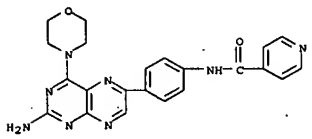


RN 847756-47-2 HCAPLUS
CN Acetamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-2-(phenylmethoxy)- (CA INDEX NAME)

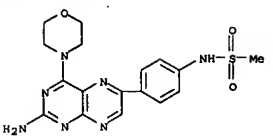


RN 847756-48-3 HCAPLUS
CN 4-Pyridinecarboxamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

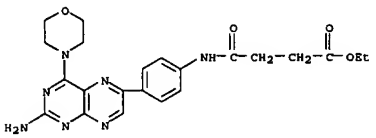


RN 847756-50-7 HCAPLUS
CN Methanesulfonamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

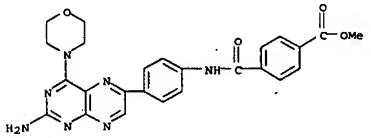
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-51-8 HCAPLUS
CN Butanoic acid, 4-[[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-4-oxo-, ethyl ester (CA INDEX NAME)

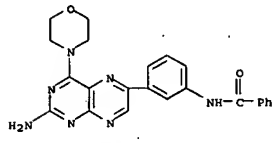


RN 847756-52-9 HCAPLUS
CN Benzoic acid, 4-[[[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

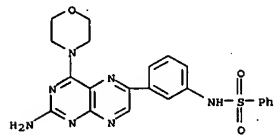


RN 847756-53-0 HCAPLUS
CN Benzamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

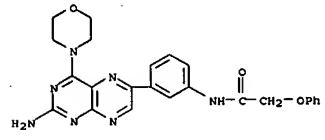
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-54-1 HCAPLUS
CN Benzenesulfonamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

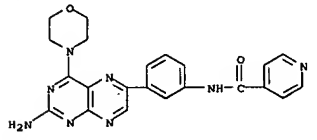


RN 847756-55-2 HCAPLUS
CN Acetamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-2-phenoxy- (CA INDEX NAME)

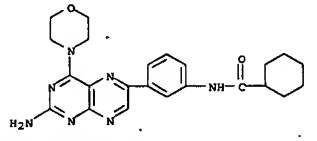


RN 847756-56-3 HCAPLUS
CN 4-Pyridinecarboxamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

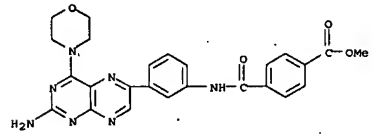
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-57-4 HCAPLUS
CN Cyclohexanecarboxamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

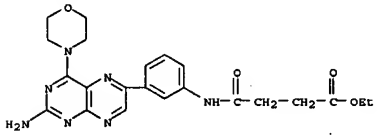


RN 847756-58-5 HCAPLUS
CN Benzoic acid, 4-[[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

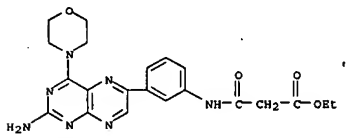


RN 847756-59-6 HCAPLUS
CN Butanoic acid, 4-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-4-oxo-, ethyl ester (CA INDEX NAME)

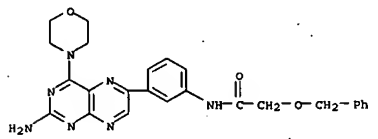
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-60-9 HCAPLUS
CN Propanoic acid, 3-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-3-oxo-, ethyl ester (CA INDEX NAME)

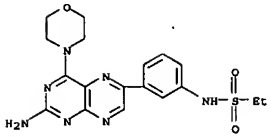


RN 847756-61-0 HCAPLUS
CN Acetamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-2-(phenylmethoxy)- (CA INDEX NAME)



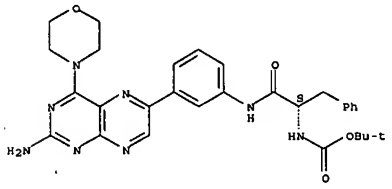
RN 847756-62-1 HCAPLUS
CN Ethanesulfonamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-63-2 HCAPLUS
CN Carbamic acid, [(1S)-2-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

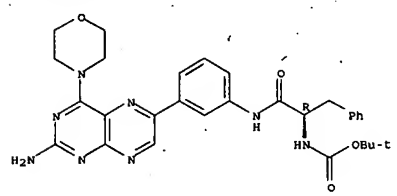
Absolute stereochemistry.



RN 847756-64-3 HCAPLUS
CN Carbamic acid, [(1R)-2-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

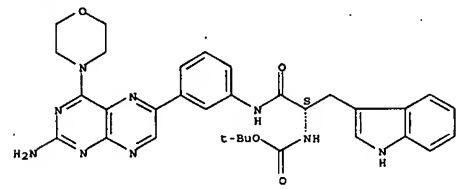
Absolute stereochemistry.

L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



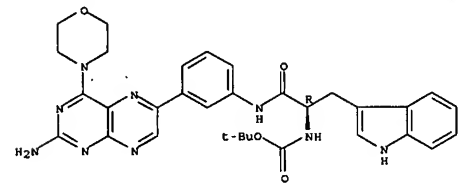
RN 847756-65-4 HCAPLUS
CN Carbamic acid, [(1S)-2-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-1-(1H-indol-3-ylmethyl)-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



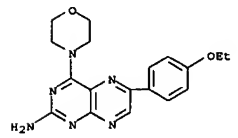
RN 847756-66-5 HCAPLUS
CN Carbamic acid, [(1R)-2-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-1-(1H-indol-3-ylmethyl)-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

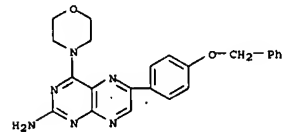


L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

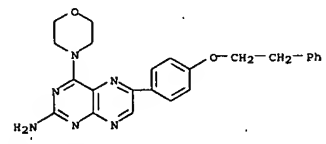
RN 847756-68-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-ethoxyphenyl)-4-(4-morpholinyl)- (CA INDEX NAME)



RN 847756-69-8 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-[4-(phenylmethoxy)phenyl]- (CA INDEX NAME)

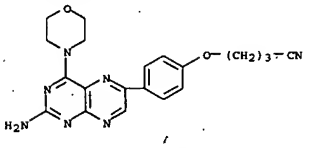


RN 847756-70-1 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-[4-(2-phenylethoxy)phenyl]- (CA INDEX NAME)

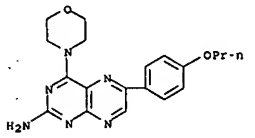


RN 847756-71-2 HCAPLUS
CN Butanenitrile, 4-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenoxy]- (CA INDEX NAME)

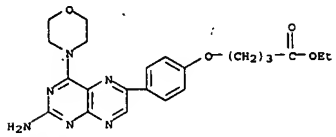
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-72-3 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-(4-propoxyphenyl)- (CA INDEX NAME)

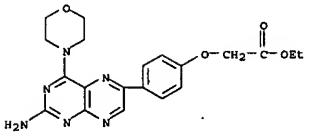


RN 847756-73-4 HCAPLUS
CN Butanoic acid, 4-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenoxy]-, ethyl ester (CA INDEX NAME)

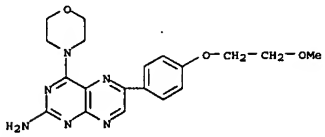


RN 847756-74-5 HCAPLUS
CN Acetic acid, [4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

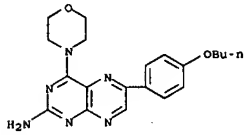
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-75-6 HCAPLUS
CN 2-Pteridinamine, 6-[4-(2-methoxyethoxy)phenyl]-4-(4-morpholinyl)- (CA INDEX NAME)

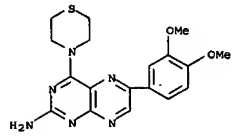


RN 847756-76-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-butoxyphenyl)-4-(4-morpholinyl)- (CA INDEX NAME)

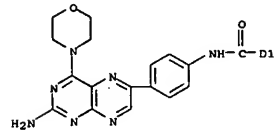


RN 847756-82-5 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(4-thiomorpholinyl)- (CA INDEX NAME)

L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

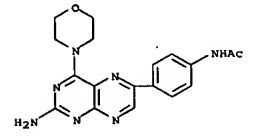


RN 848415-15-6 HCAPLUS
CN Naphthalenecarboxamide, N-[4-[2-amino-4-(4-morpholinyl)-5-pteridinyl]phenyl]- (9CI) (CA INDEX NAME)



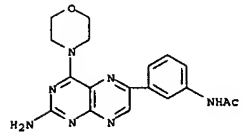
IT 847756-37-0P 847756-38-1P 847756-39-2P
847756-40-5P 847756-67-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pteridine derivs. for treatment of septic shock and TNF-α-related diseases)

RN 847756-37-0 HCAPLUS
CN Acetamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

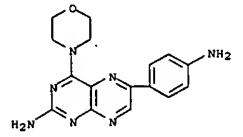


RN 847756-38-1 HCAPLUS
CN Acetamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA

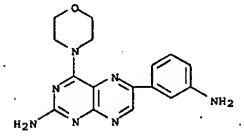
L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INDEX NAME)



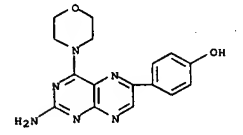
RN 847756-39-2 HCAPLUS
CN 2-Pteridinamine, 6-(4-aminophenyl)-4-(4-morpholinyl)- (CA INDEX NAME)



RN 847756-40-5 HCAPLUS
CN 2-Pteridinamine, 6-(3-aminophenyl)-4-(4-morpholinyl)- (CA INDEX NAME)

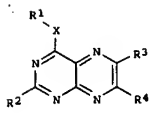


RN 847756-67-6 HCAPLUS
CN Phenol, 4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]- (CA INDEX NAME)



L8 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L8 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 16 Mar 2005
GI



I

AB This invention relates to the use of a group of pteridine derivs. I (X = O, or S(O)m wherein m is an integer from 0 to 2, or a substituted amine; R1 = alkyl, alkynyl, cycloalkyl, aryl heterocycle, halogen, alkoxy etc.; R2 = amino, acylamino, thioacylamino, carbamoyl, thiocarbamoyl, ureido, thioredio, sulfon-amido, hydroxylamino, alkoxyamino, thioalkylamino, mercaptoamino, hydrazino, alkylhydrazino, aryl, heterocycle, etc.; R3, R4 = H, halogen, alkyl, alkenyl, alkynyl, alkyl, carboxy, acetoxy, alkoxy, oxyheterocyclic, etc.) their pharmaceutically acceptable salts, N-oxides, solvates, dihydro- and tetrahydro derivs. and enantiomers, for the manufacture of a medicament for the prevention or treatment of TNF-α related disorders. Thus, 2-amino-4-isopropoxypteridine was cooled in trifluoroacetic acid and treated with 35% H2O2 to give 2-amino-4-isopropoxypteridine-N8-oxide which had a IC50 value of 4.0 μM against TNF-α. The conditions treated may be septic or endotoxic shock, toxic effects of radiotherapy, TNF-α or chemotherapeutic agents, or cachexia.

ACCESSION NUMBER: 2005:228920 HCAPLUS
DOCUMENT NUMBER: 142:297927
TITLE: Pteridine derivatives for treating TNF-alpha related disorders
INVENTOR(S): Herdewijn, Piet; Waer, Mark; De Jonghe, Steven Cesar Alfons; Yuan, Lin; El Hassane, Sefrioui
PATENT ASSIGNEE(S): 4 AZA Bioscience NV, Belg.
SOURCE: Brit. UK Pat. Appl., 72 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2405793	A	20050316	GB 2003-21384	20030912
AU 2004271721	A1	20050324	AU 2004-271721	20040913
CA 2534549	A1	20050324	CA 2004-2534549	20040913
WO 2005025574	A2	20050324	WO 2004-EP10198	20040913
WO 2005025574	A3	20050630		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

L8 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1663244	A2	20060607	EP 2004-765120	20040913
EP 1663244	B1	20070815		
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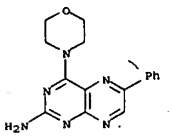
US 2007004721	A1	20070104	US 2006-595161	20060310

PRIORITY APPLN. INFO.:

GB 2003-21384	A	20030912
GB 2004-8955	A	20040422
WO 2004-EP10198	W	20040913

OTHER SOURCE(S): MARPAT 142:297927
IT 247913-58-2P 247913-59-3P 247913-60-6P
247913-61-7P 278800-06-9P 278800-07-0P
278800-08-1P 278800-09-2P 278800-18-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pteridine derivs. for treating TNF-alpha related disorders)
RN 247913-58-2 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-phenyl- (9CI) (CA INDEX NAME)



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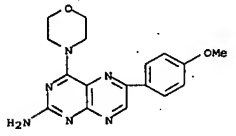
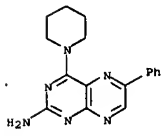
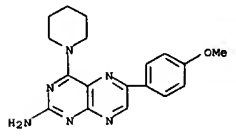
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)



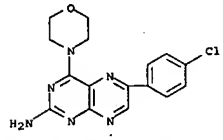
L8 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

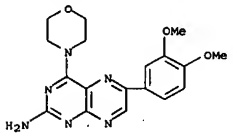


RN 278800-06-9 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

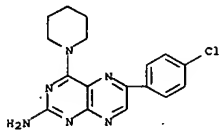


RN 278800-07-0 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

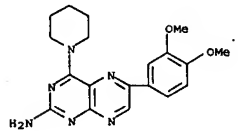
L8 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 278800-08-1 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

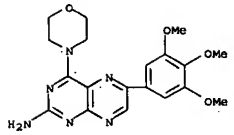


RN 278800-09-2 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 278800-18-3 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

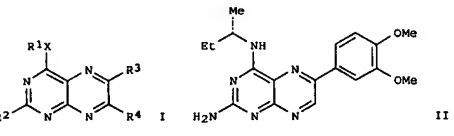
L8 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RE REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 11 Mar 2005
GI



AB This invention relates to a group of trisubstituted and tetrasubstituted pteridine derivs. I [X = O, S(O)m, NZ; m = 0-2; Z = H, OH, R1 or NZ = heterocyclic group; R1 = (un)substituted C1-7 alkyl, C2-7 alkenyl, C2-7 alkynyl, C3-10 cycloalkyl, C3-10 cycloalkenyl, aryl, alkylaryl, arylalkyl, heterocyclyl, heterocycloalkyl, etc.; R2 = amino, acylamino, thioacylamino, carbamoyl, thiocarbamoyl, ureido, thioureido, sulfonamido, hydroxylamino, alkoxyamino, thioalkylamino, hydrazino, etc.; R3 = F, Cl, Br, iodo, any group R1; R4 = H, halo, any group R1], their pharmaceutically acceptable salts, N-oxides, solvates, dihydro and tetrahydro derivs. and enantiomers, possessing unexpectedly desirable pharmaceutical properties, in particular which are highly active immunosuppressive agents, and as such are useful in the treatment in transplant rejection and/or in the treatment of certain inflammatory diseases. These compds. are also useful in preventing or treating cardiovascular disorders, allergic conditions, disorders of the central nervous system and cell proliferative disorders. Thus, (S)-sec-butylpteridine II (prepared in several steps from 2,6-diamino-5-hydroxypyrimidine, 3,4-dimethoxyphenylglyoxal oxime, and (S)-sec-butylamine) showed an IC50 of 0.2 μmol/L in a mixed lymphocyte suppression assay and an IC50 value of 0.3 μM in a TNF-α suppression assay.

ACCESSION NUMBER: 2005:216684 HCAPLUS
DOCUMENT NUMBER: 142:298130
TITLE: Preparation and immunosuppressive effects of pteridine derivatives
INVENTOR(S): Waer, Mark Jozef Albert; Herdewijn, Piet Andre Maurits Maria; Pfleiderer, Wolfgang Eugén; Marchand, Arnaud Didier Marie; De Jonghe, Steven Cesar Alfons
PATENT ASSIGNEE(S): 4 Aza Bioscience NV, Belg.
SOURCE: PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

WO 2005021003	A2	20050310	WO 2004-BE124	20040827
WO 2005021003	A3	20050609		
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004077859	A1	20040422	US 2003-651604	20030829
GB 2413324	A	20051026	GB 2004-8955	20040422
AU 2004267885	A1	20050310	AU 2004-267885	20040827
CA 2534151	A1	20050310	CA 2004-2534151	20040827
EP 1658081	A2	20060524	EP 2004-761485	20040827
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
US 2006287314	A1	20061221	US 2006-595126	20060227

PRIORITY APPLN. INFO.:

US 2003-651604	A	20030829
GB 2004-8955	A	20040422
US 1998-113989P	P	19981228
WO 1999-EP10320	W	19991228
US 2001-869468	B2	20011010
WO 2004-BE124	W	20040827

OTHER SOURCE(S): CASREACT 142:298130; MARPAT 142:298130
IT 247913-58-2P 247913-59-3P 247913-60-6P
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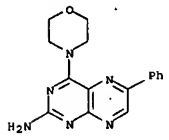
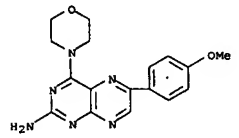
847756-72-3P 847756-73-4P 847756-74-5P
847756-75-6P 847756-76-7P 847756-82-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and immunosuppressive effects of pteridine derivs.)
RN 247913-58-2 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-phenyl- (9CI) (CA INDEX NAME)

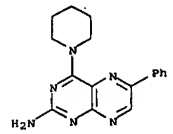
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 247913-59-3 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

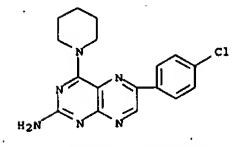


RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

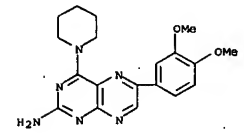


RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

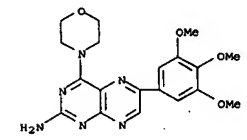
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



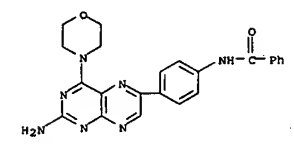
RN 278800-09-2 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



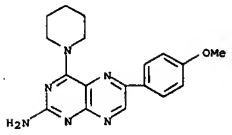
RN 278800-18-3 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



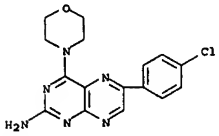
RN 847756-41-6 HCAPLUS
CN Benzamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)



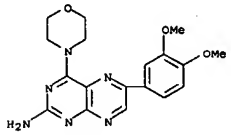
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 278800-06-9 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)



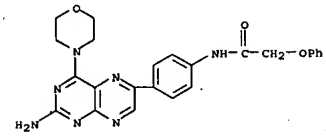
RN 278800-07-0 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)



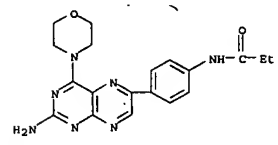
RN 278800-08-1 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

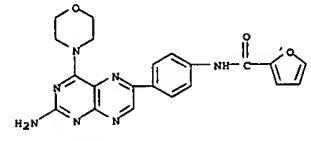
RN 847756-42-7 HCAPLUS
CN Acetamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-2-phenoxy- (CA INDEX NAME)



RN 847756-43-8 HCAPLUS
CN Propanamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

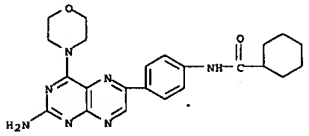


RN 847756-44-9 HCAPLUS
CN 2-Furancarboxamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

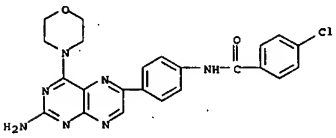


RN 847756-45-0 HCAPLUS
CN Cyclohexanecarboxamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-46-1 HCAPLUS
CN Benzamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-4-chloro- (CA INDEX NAME)



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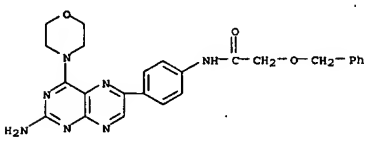
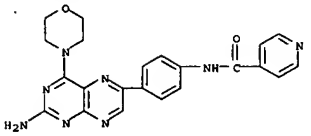
CN Acetamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-2-(phenylmethoxy)- (CA INDEX NAME)

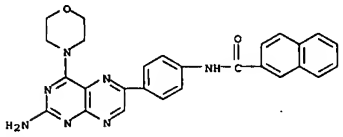


RN 847756-48-3 HCAPLUS
CN 4-Pyridinecarboxamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

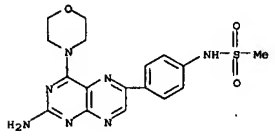
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-49-4 HCAPLUS
CN 2-Naphthalenecarboxamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

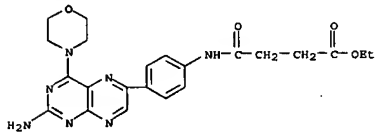


RN 847756-50-7 HCAPLUS
CN Methanesulfonamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

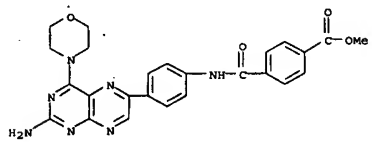


RN 847756-51-8 HCAPLUS
CN Butanoic acid, 4-[[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-4-oxo-, ethyl ester (CA INDEX NAME)

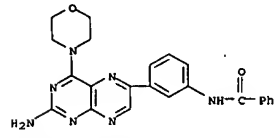
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-52-9 HCAPLUS
CN Benzoic acid, 4-[[[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

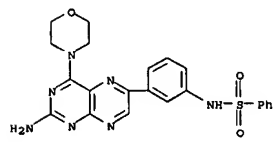


RN 847756-53-0 HCAPLUS
CN Benzamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

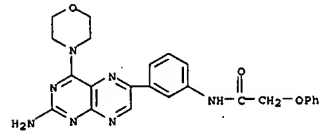


RN 847756-54-1 HCAPLUS
CN Benzenesulfonamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

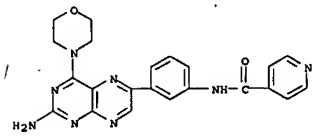
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-55-2 HCAPLUS
CN Acetamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-2-phenoxy- (CA INDEX NAME)

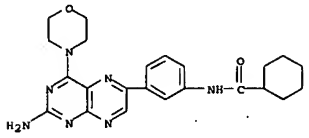


RN 847756-56-3 HCAPLUS
CN 4-Pyridinecarboxamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

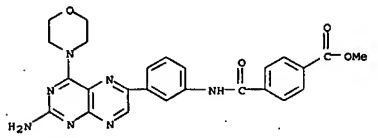


RN 847756-57-4 HCAPLUS
CN Cyclohexanecarboxamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

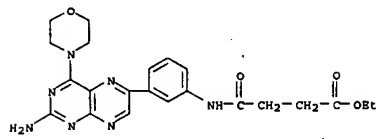
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-58-5 HCAPLUS
CN Benzoic acid, 4-[[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

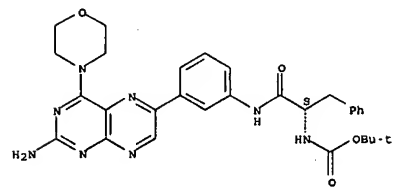


RN 847756-59-6 HCAPLUS
CN Butanoic acid, 4-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-4-oxo-, ethyl ester (CA INDEX NAME)



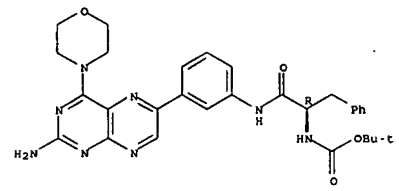
RN 847756-60-9 HCAPLUS
CN Propanoic acid, 3-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-3-oxo-, ethyl ester (CA INDEX NAME)

L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



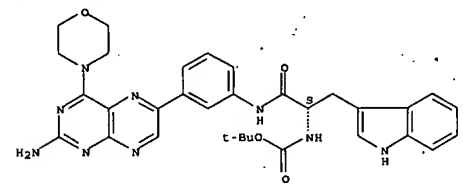
RN 847756-64-3 HCAPLUS
CN Carbamic acid, [(1R)-2-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

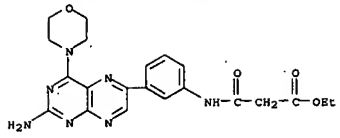


RN 847756-65-4 HCAPLUS
CN Carbamic acid, [(1S)-2-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-1-(1H-indol-3-ylmethyl)-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

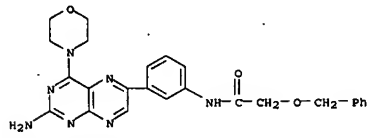
Absolute stereochemistry.



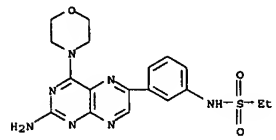
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-61-0 HCAPLUS
CN Acetamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]-2-(phenylmethoxy)- (CA INDEX NAME)



RN 847756-62-1 HCAPLUS
CN Ethanesulfonamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)



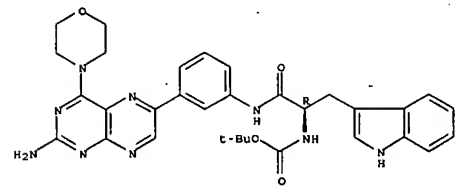
RN 847756-63-2 HCAPLUS
CN Carbamic acid, [(1S)-2-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

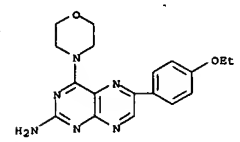
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 847756-66-5 HCAPLUS
CN Carbamic acid, [(1R)-2-[[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]amino]-1-(1H-indol-3-ylmethyl)-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

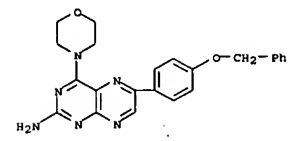
Absolute stereochemistry.



RN 847756-68-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-ethoxyphenyl)-4-(4-morpholinyl)- (CA INDEX NAME)

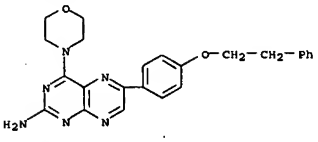


RN 847756-69-8 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-[4-(phenylmethoxy)phenyl]- (CA INDEX NAME)

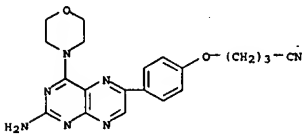


RN 847756-70-1 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-[4-(2-phenylethoxy)phenyl]- (CA INDEX NAME)

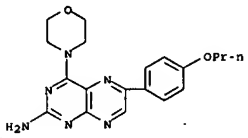
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-71-2 HCAPLUS
CN Butanenitrile, 4-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenoxy]-(CA
INDEX NAME)

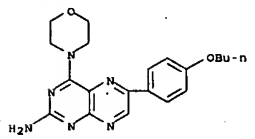


RN 847756-72-3 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-(4-propoxyphenyl)- (CA INDEX NAME)

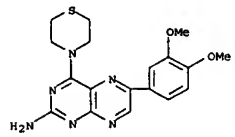


RN 847756-73-4 HCAPLUS
CN Butanoic acid, 4-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenoxy]-, ethyl ester (CA INDEX NAME)

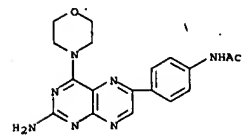
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-82-5 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(4-thiomorpholinyl)- (CA INDEX
NAME)

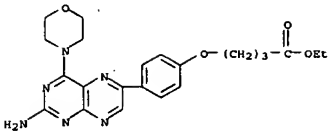


IT 847756-37-0P 847756-38-1P 847756-39-2P
847756-40-5P 847756-67-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and immunosuppressive effects of pteridine derivs.)
RN 847756-37-0 HCAPLUS
CN Acetamide, N-[4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

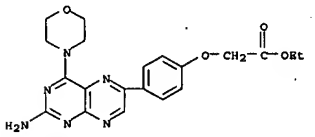


RN 847756-38-1 HCAPLUS
CN Acetamide, N-[3-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenyl]- (CA INDEX NAME)

L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 847756-74-5 HCAPLUS
CN Acetic acid, [4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)



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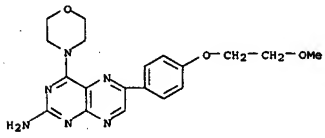
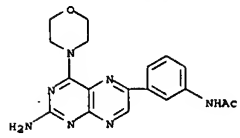
CN 2-Pteridinamine, 6-[4-(2-methoxyethoxy)phenyl]-4-(4-morpholinyl)- (CA INDEX NAME)

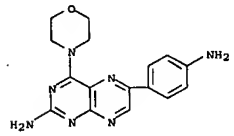


RN 847756-76-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-butoxyphenyl)-4-(4-morpholinyl)- (CA INDEX NAME)

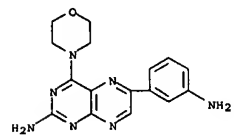
L8 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



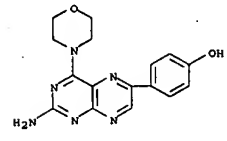
RN 847756-39-2 HCAPLUS
CN 2-Pteridinamine, 6-(4-aminophenyl)-4-(4-morpholinyl)- (CA INDEX NAME)



RN 847756-40-5 HCAPLUS
CN 2-Pteridinamine, 6-(3-aminophenyl)-4-(4-morpholinyl)- (CA INDEX NAME)



RN 847756-67-6 HCAPLUS
CN Phenol, 4-[2-amino-4-(4-morpholinyl)-6-pteridinyl]- (CA INDEX NAME)



L8 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Apr 2004
AB This invention relates to a group of trisubstituted and tetrasubstituted pteridine derivs., their pharmaceutically acceptable salts, N-oxides, solvates, dihydro- and tetrahydroderivatives and enantiomers, possessing unexpectedly desirable pharmaceutical properties, in particular which are highly active immunosuppressive agents, and as such are useful in the treatment in transplant rejection and/or in the treatment of certain inflammatory diseases. These compds. are also useful in preventing or treating cardiovascular disorders, allergic conditions, disorders of the central nervous system and cell proliferative disorders. The pteridine derivs. (preparation given) inhibited the mixed lymphocyte reaction and reduced
T cell proliferation in the CD3 and CD28 assay.
ACCESSION NUMBER: 2004:331825 HCAPLUS
DOCUMENT NUMBER: 140:350561
TITLE: Immunosuppressive effects of pteridine derivatives and
pharmaceutical compositions containing them
INVENTOR(S): Waer, Mark Jozef Albert; Herdewijn, Piet Andre Maurits
Maria; Pfleiderer, Wolfgang Eugen
PATENT ASSIGNEE(S): Belg.
SOURCE: U.S. Pat. Appl. Publ., 46 pp., Cont.-in-part of U.S. Ser. No. 869,468, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004077859	A1	20040422	US 2003-651604	20030829
WO 2000039129	A1	20000706	WO 1999-EP10320	19991228
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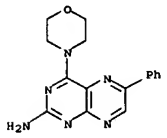
US 2006287314	A1	20061221	US 2006-595126	20060227

PRIORITY APPLN. INFO.:

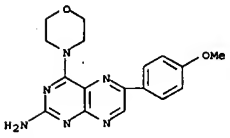
US 1998-113989P	P	19981228
WO 1999-EP10320	W	19991228
US 2001-869468	B2	20011010
US 2003-651604	A	20030829
GB 2004-8955	A	20040422
WO 2004-BE124	W	20040827

OTHER SOURCE(S): MARPAT 140:350561
IT 247913-58-2P 247913-59-3P 247913-60-6P
247913-61-7P 278800-06-9P 278800-07-0P
278800-08-1P 278800-09-2P 278800-18-3P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(immunosuppressant pteridine derivs. and compns.)
RN 247913-58-2 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-phenyl- (9CI) (CA INDEX NAME)

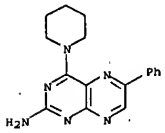


RN 247913-59-3 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

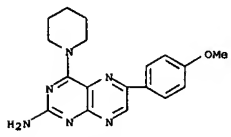
L8 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



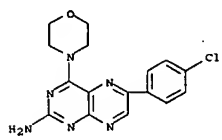
RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

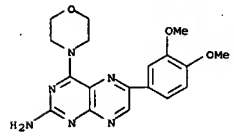


RN 278800-06-9 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

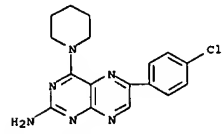


L8 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

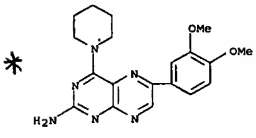
RN 278800-07-0 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)



RN 278800-08-1 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

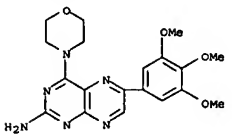


RN 278800-09-2 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 278800-18-3 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 26 May 2002

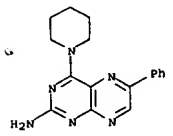
AB The family of homodimeric nitric oxide synthases (NOS I-III) catalyzes the generation of the cellular messenger nitric oxide (NO) by oxidation of the substrate L-arginine. The rational design of specific NOS inhibitors is of therapeutic interest in regulating pathol. NO levels associated with sepsis, inflammatory, and neurodegenerative diseases. The cofactor (6R)-5,6,7,8-tetrahydrobiopterin (H4Bip) maximally activates all NOSs and stabilizes enzyme quaternary structure by promoting and stabilizing dimerization. Here, we describe the synthesis and three-dimensional (3D) quant. structure-activity relationship (QSAR) anal. of 65 novel 4-amino- and 4-oxo-pteridines (antipterins) as inhibitors targeting the H4Bip binding site of the neuronal NOS isoform (NOS-I). The exptl. binding modes for two inhibitors complexed with the related endothelial NO synthase (NOS-III) reveal requirements of biol. affinity and form the basis for ligand alignment. Different alignment rules were derived by building other compds. accordingly using manual superposition or a genetic algorithm for flexible superposition. Those alignments led to 3D-QSAR models (comparative mol. field anal. (CoMFA) and comparative mol. similarity index anal. (CoMSIA)), which were validated using leave-one-out cross-validation, multiple analyses with two and five randomly chosen cross-validation groups, perturbation of biol. activities by randomization or progressive scrambling, and external prediction. An iterative realignment procedure based on rigid field fit was used to improve the consistency of the resulting partial least squares models. This led to consistent and highly predictive 3D-QSAR models with good correlation coeffs. for both CoMFA and CoMSIA, which correspond to exptl. determined NOS-II and -III H4Bip binding site topologies as well as to the NOS-I homol. model binding site in terms of steric, electrostatic, and hydrophobic complementarity. These models provide clear guidelines and accurate activity predictions for novel NOS-I inhibitors.

ACCESSION NUMBER: 2002:392358 HCAPLUS
DOCUMENT NUMBER: 137:119060
TITLE: Structural Requirements for Inhibition of the Neuronal Nitric Oxide Synthase (NOS-I): 3D-QSAR Analysis of 4-Oxo- and 4-Amino-Pteridine-Based Inhibitors
AUTHOR(S): Matter, Hans; Kotsonis, Peter; Klingler, Otmar; Strobel, Hartmut; Proehlich, Lothar G.; Frey, Armin; Pfleiderer, Wolfgang; Schmidt, Harald H. H. W.
CORPORATE SOURCE: Molecular Modeling, Aventis Pharma, Frankfurt am Main, 65926, Germany
SOURCE: Journal of Medicinal Chemistry (2002), 45(14), 2923-2941
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:119060

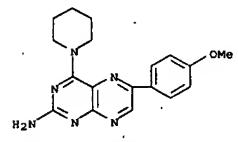
L8 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 247913-60-6 247913-61-7
RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(preparation and QSAR of 4-oxo- and 4-amino-pteridine-based neuronal NOS inhibitors)

RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



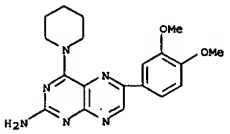
RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



IT 278800-09-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and QSAR of 4-oxo- and 4-amino-pteridine-based neuronal NOS inhibitors)

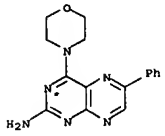
RN 278800-09-2 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

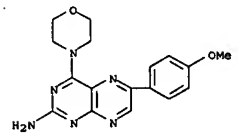


IT 247913-58-2 247913-59-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation and QSAR of 4-oxo- and 4-amino-pteridine-based neuronal NOS inhibitors)

RN 247913-58-2 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-phenyl- (9CI) (CA INDEX NAME)



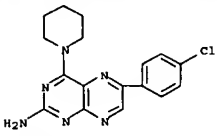
RN 247913-59-3 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)



IT 278800-08-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and QSAR of 4-oxo- and 4-amino-pteridine-based neuronal NOS inhibitors)

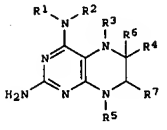
RN 278800-08-1 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

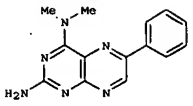


REFERENCE COUNT: 111 THERE ARE 111 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 30 Mar 2001
GI



I



II

AB Pteridines, such as I [R1, R2 = H, alkyl, aryl, arylalkyl; R1R2 = nitrogen bound heterocyclyl, such as 1-piperidinyl or 4-morpholinyl; R4 = alkyl, alkenyl, alkynyl, cycloalkenyl, aryl, etc.; R3, R5 = acyl, aroyl, R6 = R7 = H, or R3R6 = R5R7 = bond;], were prepared for pharmaceutical use.
Thus, pteridine II was prepared via cyclocondensation of N4,N4-dimethylpyrimidinetetramine dihydrochloride and phenylglyoxal monoxime. The prepared pteridines were tested for nitric oxide synthase inhibiting activity.

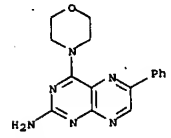
ACCESSION NUMBER: 2001:228889 HCAPLUS
DOCUMENT NUMBER: 134:237499
TITLE: Preparation of N-substituted-4-aminopteridines as NO synthase inhibitors for use as pharmaceuticals
INVENTOR(S): Pfleiderer, Wolfgang; Schmidt, Harald; Froehlich, Lothar; Kotsonis, Peter; Taghavi-Moghadam, Shahriyar
PATENT ASSIGNEE(S): Vasopharm Biotech G.m.b.H. & Co. K.-G., Germany
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001021619	A1	20010329	WO 2000-EP8833	20000911
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19944767	A1	20010329	DE 1999-19944767	19990917

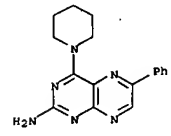
L8 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

EP 1216246	A1	20020626	EP 2000-964154	20000911
EP 1216246	B1	20050824		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2004522690	T	20040729	JP 2001-524995	20000911
AT 302778	T	20050915	AT 2000-964154	20000911
ES 2248124	T3	20060316	ES 2000-964154	20000911
US 6844343	B1	20050118	US 2002-70976	20020719
PRIORITY APPLN. INFO.:			DE 1999-19944767	A 19990917
			WO 2000-EP8833	W 20000911

OTHER SOURCE(S): MARPAT 134:237499
IT 247913-58-2P 247913-60-6P 247913-61-7P
278800-07-0P 278800-08-1P 330575-33-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of N-substituted-4-aminopteridines as NO synthase inhibitors for pharmaceutical use)
RN 247913-58-2 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-phenyl- (9CI) (CA INDEX NAME)

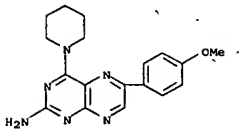


RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

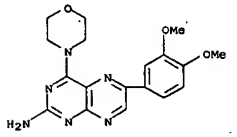


RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

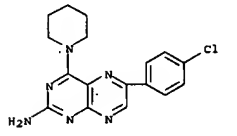
L8 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 278800-07-0 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

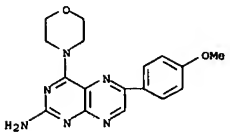


RN 278800-08-1 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



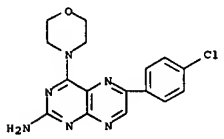
RN 330575-33-2 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(4-morpholinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

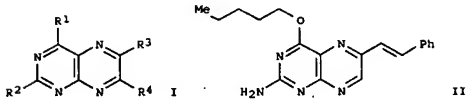
IT 330575-32-1P 330575-34-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-substituted-4-aminopteridines as NO synthase inhibitors
for pharmaceutical use)
RN 330575-32-1 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(4-morpholinyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 330575-34-3 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(1-piperidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L8 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 07 Jul 2000
GI



AB Pteridines, such as I (R1, R2 = NH2, NHOH, alkylamine, dialkylamine, alkyloxyamine, dialkyloxyamine, nitrogen containing heterocyclyl, etc.; R3 = halogen, alkoxy, alkyl, aryl, etc.; R4 = H, alkyl, alkoxy, aryl) were prepared for pharmaceutical use in the treatment of inflammatory diseases and autoimmune disorders. Thus, pteridine II was prepared in 72% yield by reaction of 6-chloro-4-(pentyloxy)-2-pteridinamine and styrene using palladium acetate, tri-o-tolylphosphine, cuprous iodide, and triethylamine in acetonitrile. The prepared pteridines were tested for immunosuppressive and anti-inflammatory activity.

ACCESSION NUMBER: 2000:457070 HCAPLUS
DOCUMENT NUMBER: 133:73895
TITLE: Preparation of pteridine derivatives for pharmaceutical use in the treatment of inflammatory diseases and autoimmune disorders
INVENTOR(S): Waer, Mark Joseph Albert; Herdewijn, Piet Andre Maurits Maria; Pfleiderer, Wolfgang Eugen
PATENT ASSIGNEE(S): K.U. Leuven Research & Development, Belg.
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039129	A1	20000706	WO 1999-EP10320	19991228
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2356380	A1	20000706	CA 1999-2356380	19991228
EP 1144412	A1	20011017	EP 1999-964663	19991228
EP 1144412	B1	20040929		
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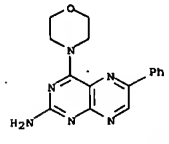
JP 2002533464	T	20021008	JP 2000-591040	19991228
AU 770551	B2	20040226	AU 2000-30429	19991228
AT 277929	T	20041015	AT 1999-964663	19991228
ES 2229803	T3	20050416	ES 1999-964663	19991228
US 2004077859	A1	20040422	US 2003-651604	20030829
US 2006189620	A1	20060824	US 2006-275601	20060118
US 2006287314	A1	20061221	US 2006-595126	20060227

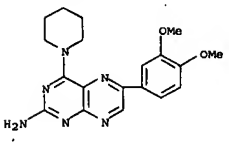
PRIORITY APPLN. INFO.: US 1998-113989P P 19981228
WO 1999-EP10320 W 19991228
US 2001-869468 B2 20011010
US 2003-651604 A1 20030829
GB 2004-8955 A 20040422
WO 2004-BE124 W 20040827

OTHER SOURCE(S): MARPAT 133:73895
IT 247913-58-2P 247913-59-3P 247913-60-6P
247913-61-7P 278800-06-9P 278800-07-0P
278800-08-1P 278800-09-2P 278800-18-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pteridine derivs. for pharmaceutical use in the treatment of
inflammatory diseases and autoimmune disorders)
RN 247913-58-2 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-phenyl- (9CI) (CA INDEX NAME)



RN 247913-59-3 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

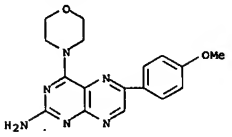
L8 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



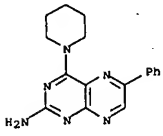
● HCl

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

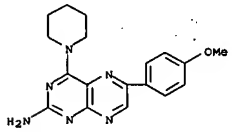
L8 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

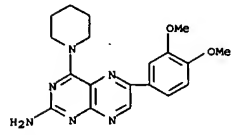


RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

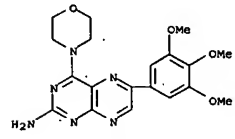


RN 278800-06-9 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



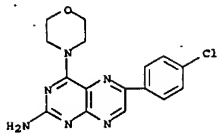
RN 278800-18-3 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



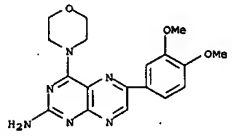
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

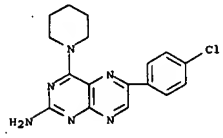
L8 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 278800-07-0 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)



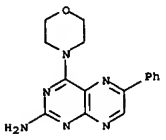
RN 278800-08-1 HCAPLUS
CN 2-Pteridinamine, 6-(4-chlorophenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



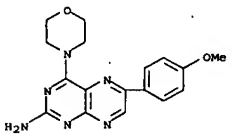
RN 278800-09-2 HCAPLUS
CN 2-Pteridinamine, 6-(3,4-dimethoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 21 Sep 1999
AB The family of nitric oxide synthases (NOS) catalyzes the conversion of L-arginine to L-citrulline and nitric oxide (NO), an important cellular messenger mol. which has been implicated in the pathophysiol. of septic shock and inflammatory and neurodegenerative disease states. NOS can be maximally activated by the ubiquitous cofactor, (6R)-5,6,7,8-tetrahydrobiopterin (H4Bip), and antagonists of H4Bip may be of therapeutic importance to inhibit pathol. high NO formation. The 4-amino substituted analog of H4Bip was reported to be a potent NOS inhibitor. Therefore, we developed a series of novel 4-amino pteridine derivs., anti-pterins, to pharmacol. target the neuronal isoform of nitric oxide synthase (NOS-I). To functionally characterize the pterin/anti-pterin interaction and establish a structure-activity relationship (SAR), we systematically altered the substituents in the 2-, 4-, 5-, 6-, and 7-position of the pteridine nucleus. Varying the substitution pattern in the 2-, 5-, and 7-position resulted in no significant inhibitory effect on enzyme activity. In contrast, bulky substituents in the 6-position, such as Ph, markedly increased the inhibitory potency of the reduced 4-amino-5,6,7,8-tetrahydropteridines, possibly as a consequence of hydrophobic interactions within NOS-I. However, this was not the case for the aromatic 4-amino pteridines. Interestingly, chemical modification of the 4-amino substituent by dialkyl/diaralkylation together with 6-arylation of the aromatic 2,4-diamino pteridine resulted in potent and efficacious inhibitors of NOS-I, suggesting possible hydrophilic and hydrophobic interactions within NOS-I. This SAR agrees with (a) the recently published crystal structure of the oxygenase domain of the inducible NOS isoform (NOS-II) and (b) the comparative mol. field anal. of selected NOS-I inhibitors, which resulted in a 3D-QSAR model of the pterin binding site interactions. Further optimization should be possible when the full length structure of NOS-I becomes available.
ACCESSION NUMBER: 1999:589097 HCAPLUS
DOCUMENT NUMBER: 131:317316
TITLE: Inhibition of Neuronal Nitric Oxide Synthase by 4-Amino Pteridine Derivatives: Structure-Activity Relationship of Antagonists of (6R)-5,6,7,8-Tetrahydrobiopterin Cofactor
AUTHOR(S): Proehlich, Lothar G.; Kotsonis, Peter; Traub, Hermann; Taghavi-Moghadam, Shahriyar; Al-Masoudi, Najim; Hofmann, Heinrich; Strobel, Hartmut; Matter, Hans; Pfleiderer, Wolfgang; Schmidt, Harald H. H. W.
CORPORATE SOURCE: Department of Pharmacology and Toxicology, Julius-Maximilians University Wuerzburg, Wuerzburg, 97078, Germany
SOURCE: Journal of Medicinal Chemistry (1999), 42(20), 4108-4121
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 247913-58-2P 247913-59-3P 247913-60-6P
247913-61-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

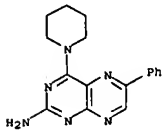
L8 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Uses)
(synthesis of and inhibition of neuronal nitric oxide synthase by aminopteridines)
RN 247913-58-2 HCAPLUS
CN 2-Pteridinamine, 4-(4-morpholinyl)-6-phenyl- (9CI) (CA INDEX NAME)



RN 247913-59-3 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)

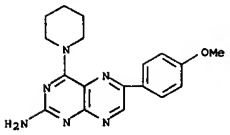


RN 247913-60-6 HCAPLUS
CN 2-Pteridinamine, 6-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



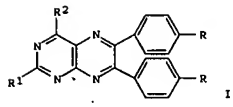
RN 247913-61-7 HCAPLUS
CN 2-Pteridinamine, 6-(4-methoxyphenyl)-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



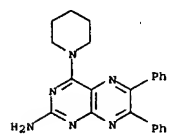
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
GI

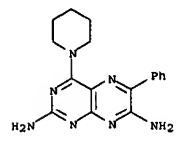


I

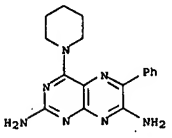
AB Diarylpteridines (I, R = H, OMe, OEt, R1 = MeS, NH2, R2 = OH) were obtained in 70-82.5% yields by condensation of the corresponding diaminopyrimidine with p-RC6H4COCOC6H4-p 3 hr in boiling AcOH-EtOH. Chlorination of I (R = H, R1 = NH2, R2 = OH) with PCl5 gave 71% I (R2 = Cl). Substitution reactions of the latter gave 45.6-70.5% I (R2 = EtO, Me2N, Et2N, piperidino, NHNH2).
ACCESSION NUMBER: 1976:560035 HCAPLUS
DOCUMENT NUMBER: 85:160035
TITLE: Pteridine derivatives. I. Synthesis of some substituted 6,7-diarylpteridines
AUTHOR(S): Kaldrikyan, M. A.; Danagulyan, G. G.; Khekoyan, A. V.;
Arsenyan, F. G.; Aroyan, A. A.
CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
SOURCE: Armyanskii Khimicheskii Zhurnal (1976), 29(4), 337-41
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT 60783-57-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 60783-57-5 HCAPLUS
CN 2-Pteridinamine, 6,7-diphenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB A number of 4,7-diamino-6-phenyl-, 2,7-diamino-6-phenyl- and 2,4,7-triamino-6-arylpteridines were prepared for diuretic testing by condensation of arylacetonitriles and 4-amino-5-nitrosopyrimidines. 2,4-Diamino-6-(methylthio)-5-nitrosopyrimidine and 4,6-diamino-2-(methylthio)-5-nitrosopyrimidine were treated with amines to give replacement of the MeS group by an amino group. Uv and N.M.R. spectra suggest that the 2-cyanomethyl- and 2-carboxamidomethyl-4,7-diamino-6-phenylpteridines exist as tautomers in which the cyano and carboxamido groups are conjugated with the pteridine ring. Certain other conclusions were drawn from the spectral data. 20 references.
ACCESSION NUMBER: 1968:467335 HCAPLUS
DOCUMENT NUMBER: 69:67335
TITLE: Pteridines. VI. Preparation of some 6-aryl-7-aminopteridines
AUTHOR(S): Weinstock, Joseph; Dunoff, Roberta Y.; Sutton, Blaine;
Trost, Barry; Kirkpatrick, Joel; Farina, Frank; Straub, Alice S.
CORPORATE SOURCE: Res. and Develop. Div., Smith Kline and French Lab., Philadelphia, PA, USA
SOURCE: Journal of Medicinal Chemistry (1968), 11(3), 549-56
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 19173-02-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19173-02-5 HCAPLUS
CN Pteridine, 2,7-diamino-6-phenyl-4-piperidino- (8CI) (CA INDEX NAME)



L8 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
AB The diuretic activity of pteridines related to 2,4,7-triamino-6-phenylpteridine (triamterene), 2,4-diamino-6,7-dimethylpteridine (I), and 4,7-diamino-2-phenyl-pteridine-6-carboxamide was studied in the saline-loaded and sodium-deficient rat. A limited number of related pyrimidopyrimidines were similarly studied. Some of the compds. related to triamterene and I not only cause Na+ excretion but also conserve K+. All the 2-phenylpteridines that were studied which are active natriuretic agents also cause K+ excretion. In the triamterene series, replacement of any of the amino groups by either a large amine or a nonbasic group other than H leads to reduction of diuretic activity. Replacement of the Ph by a small, nonbasic group gives active diuretic agents, but an aromatic (or heteroaromatic) group seems desirable for highest activity. Some variation in the substitution pattern on the pteridine ring is permissible as demonstrated by the activity of the triamterene isomers. The 7-Ph isomer is outstanding as a blocker of K+ excretion.
ACCESSION NUMBER: 1968:452104 HCAPLUS
DOCUMENT NUMBER: 69:52104
TITLE: Pteridines. XII. Structure-activity relation of some pteridine diuretics
AUTHOR(S): Weinstock, Joseph; Wilson, James W.; Wiebelhaus, Virgil D.; Maass, Alfred R.; Brennan, Francis T.; Sosnowski, Genevieve
CORPORATE SOURCE: Res. and Develop. Div., Smith Kline and French Lab., Philadelphia, PA, USA
SOURCE: Journal of Medicinal Chemistry (1968), 11(3), 573-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 19173-02-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(as diuretic)
RN 19173-02-5 HCAPLUS
CN Pteridine, 2,7-diamino-6-phenyl-4-piperidino- (8CI) (CA INDEX NAME)

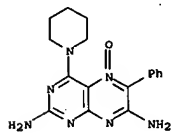


L8 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB A process which circumvents the standard methods of preparing N-oxide derivs., which would lead to degradation of the pteridine nucleus of title compds., is described. The process is carried out by treating a pyridinium reagent [prepared in situ from an α-halo or benzenesulfonyl ketone and C5H5N or from an aldehyde, NaCN, PhSO2Cl (I), and C5H5N] with an appropriately substituted 6-amino-5-nitrosopyrimidine in the presence of a basic condensing agent. Condensing agents which contain CN- can be used only in reactions using the latter type of pyridinium reagent in preparing 7-aminopteridine 5-oxides. Thus, a mixture of 7.4 g. α-cyanobenzyl benzenesulfonate (II) (prepared from BzH, NaCN, and I), 8 ml. C5H5N, and 15 ml. Me2CO is refluxed 15 min., added to a solution of 4.3 g. 4,6-diamino-5-nitroso-2-phenylpyrimidine (III) in 250 ml. Me2CO followed by a solution of 2 g. NaCN in 20 ml. H2O, warmed 5 min. at 40° and kept 1 hr. at room temperature to give 4,7-diamino-2,6-diphenylpteridine 5-oxide, m. 355°. A mixture of 21.5 g. III, 20 g. KOAc, 25.6 g. acetonylpyridinium chloride (IV), 100 ml. H2O, and 1 l. EtOH is refluxed 1 hr. to give 4-amino-7-methyl-2-phenylpteridine 5-oxide, m. 287° (decomposition). Similarly prepared (pyridinium reagent, substituents on 5-nitrosopyrimidine, condensing agent, and product given) are: II and C5H5N, 4,6-diamino-2-methylthio, NaCN, 4,7-diamino-2-methylthio-6-phenylpteridine 5-oxide, m. 351° (decomposition); IV, 4,6-diamino, KOAc, 4-amino-7-methylpteridine 5-oxide, m. 250-1° (decomposition); phenacylpyridinium bromide, 4,6-diamino-2-phenyl, KOAc, 4-amino-2,7-diphenylpteridine 5-oxide, m. 258-60°; propiophenone-α-pyridinium bromide, 2,6-diamino-4-methyl, NaOAc, 2-amino-4,6-dimethyl-7-phenylpteridine 5-oxide; II and lutidine, 2-(α-thienyl)-4,6-diamino, Na2CO3, 2-(α-thienyl)-4,7-diamino-6-phenylpteridine 5-oxide; II and C5H5N, 2-methyl-4-hydroxy-6-amino, NaCN, 2-methyl-4-hydroxy-6-phenyl-7-aminopteridine 5-oxide; II and C5H5N, 2,6-diamino-4-methylthio, NaCN, 2,7-diamino-4-methylthio-6-phenylpteridine 5-oxide (V), m. 306-8° (decomposition). III, 0.5 g. of the pyridinium salt of BrCH2CONH2, and 0.5 g. KOAc in 50 ml. EtOH refluxed gives 4-amino-7-hydroxy-6-phenylpteridine 5-oxide, m. 251-2°. Diacetylated 2,4,6-triamino-5-nitrosopyrimidine (10 g.) in 120 ml. Me2SO is diluted in rapid succession with 500 ml. Me2CO, with a solution of 16.6 g. II, 16.6 ml. C5H5N, and 30 ml. heated Me2CO, and finally with 4.1 g. NaCN in 40 ml. H2O to give the diacetylaminopteridine derivative, which is then hydrolyzed with MeONa in MeOH to give 2,4,7-triamino-6-phenylpteridine 5-oxide, m. 340° (decomposition). V refluxed in piperidine for 16 hrs. gives 2,7-diamino-4-piperidino-6-phenylpteridine 5-oxide, m. 250-2° (decomposition) (EtOH). These compds. have antifolic acid activity against various microorganisms. Certain members of the series also have diuretic or antihypertensive activity.
ACCESSION NUMBER: 1965:36875 HCAPLUS
DOCUMENT NUMBER: 62:36875
ORIGINAL REFERENCE NO.: 62:6496g-h,6497a-d
TITLE: Pteridine 5-oxides

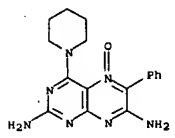
L8 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INVENTOR(S): Pachter, Irwin J.; Weinstock, Joseph
PATENT ASSIGNEE(S): Smith Kline & French Laboratories
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3159628		19641201	US 1962-197909	19620528
PRIORITY APPLN. INFO.:			US	19620528

IT 1048-67-5P, Pteridine, 2,7-diamino-6-phenyl-4-piperidino-, 5-oxide
RL: PREP (Preparation)
(preparation of)
RN 1048-67-5 HCAPLUS
CN Pteridine, 2,7-diamino-6-phenyl-4-piperidino-, 5-oxide (7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 2001
AB 4-Amino-5-nitrosopyrimidines condense with benzoylacetonitrile, phenacylpyridinium bromide, and acetonylpyridinium chloride in the presence of sodium cyanide to produce 7-amino-6-pteridyl ketones (I). Reduction of the products with sodium borohydride yields the corresponding carbinols. 7-Substituted pteridine 5-oxides are produced when 4-amino-5-nitrosopyrimidines condense with the aforementioned pyridinium salts in the presence of potassium acetate. The use of α-cyanobenzylpyridinium salts in related reactions results in the formation of 7-amino-6-phenylpteridine 5-oxides.
ACCESSION NUMBER: 1963:73306 HCAPLUS
DOCUMENT NUMBER: 58:73306
ORIGINAL REFERENCE NO.: 58:12546d-f
TITLE: Pteridines. III. Synthesis of some ketones, carbinols, and N-oxides
AUTHOR(S): Pachter, Irwin J.; Nemeth, Piroska E.; Villani, Anthony J.
CORPORATE SOURCE: Smith, Kline & French Labs., Philadelphia, PA
SOURCE: Journal of Organic Chemistry (1963), 28, 1197-202
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:73306
IT 1048-67-5P, Pteridine, 2,7-diamino-6-phenyl-4-piperidino-, 5-oxide
RL: PREP (Preparation)
(preparation of)
RN 1048-67-5 HCAPLUS
CN Pteridine, 2,7-diamino-6-phenyl-4-piperidino-, 5-oxide (7CI, 8CI) (CA INDEX NAME)



22/10/2007,10595126-lls.trn

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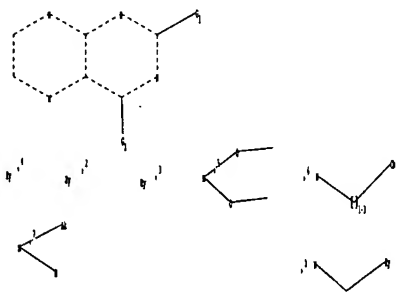
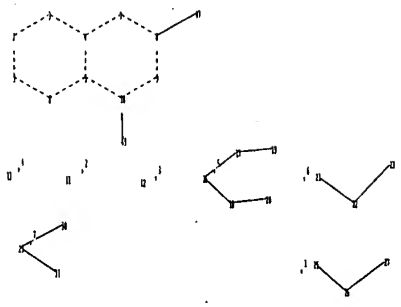
Uploading C:\Program Files\Stnexp\Queries\10595126-lls.str



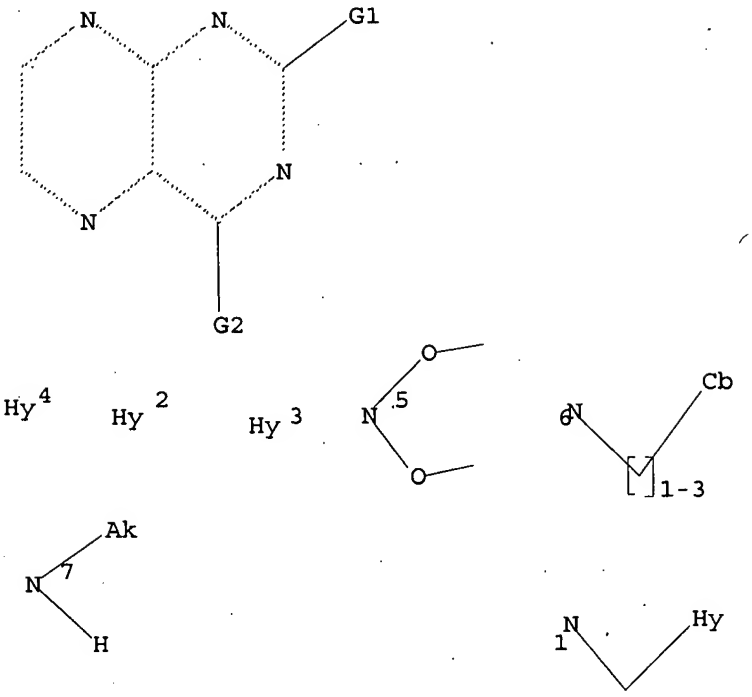


L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 NH2,[@1]

G2 [@2],[@3],[@4],[@5],[@6],[@1],[@7]

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 11:44:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     1499 TO ITERATE

100.0% PROCESSED     1499 ITERATIONS                          8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        27658 TO    32302
PROJECTED ANSWERS:               8 TO      329

L3             8 SEA SSS SAM L1

=> d scan
```